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Liquid Organic Hydrogen Carriers: Thermophysical and Thermochemical Studies of Carbazole Partly and Fully Hydrogenated Derivatives

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Abstract

© 2015 American Chemical Society. Carbazole derivatives are promising liquid organic hydrogen carrier (LOHCs). They can take up and release hydrogen in catalytic hydrogenation/dehydrogenation reactions. The thermophysical properties (heat capacity, density, viscosity, surface tension, and refractive index) of carbazole and N-ethylcarbazole, as well as those of their hydrogenated derivatives, were measured. Furthermore, thermochemical properties (enthalpy of vaporization, sublimation, and fusion) were derived from experiments. Molar enthalpies of formation of the gaseous carbazole derivatives were calculated and validated with high-level quantum chemical calculations. Molar enthalpies of formation data in the liquid phase were derived by combining the high-level quantum chemistry values of the gas-phase enthalpies of formation with experimentally determined enthalpies of vaporization. Thermodynamic analysis of the hydrogenation/dehydrogenation reactions of the carbazole derivatives was performed. This analysis, among others, revealed a rather weak dependence of thermodynamic hydrogen release characteristics on the alkyl chain length. The thermophysical properties of the derivatives show a strong dependence on the degree of hydrogenation. Therefore, the state of hydrogenation should always be considered when dealing with substance properties of LOHCs. Using the data presented in this work, a more reliable process modeling is possible.

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